

INTERACTION FINGERPRINT ANNOTATIONS FROM PROTEINSTRUCTURE MODELS

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Abstract of the Disclosure

A system and methods for rapidly and accurately assessing ligand binding characteristics for diverse classes of protein molecules. Modeling methods are used to represent the protein molecules and simulate their interaction with ligand molecules. Protein/ligand interactions are characterized by a fingerprint analysis that permits grouping of the proteins based on predicted structural features and ligand reactivity rather than sequence similarities or homology alone.

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